(i) inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence; and

(ii) by way of executable code, directing the processor to produce from the alignment a three dimensional reduced protein model comprising representations of side chains of amino acid residues comprising a target protein, wherein said representations of side chains of amino acid residues are converted to interaction centers, and each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and each interaction center is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain, which is projected onto an underlying cubic lattice to produce a projected chain of interaction centers, and then secondary constraints and/or tertiary constraints are applied to a subset of, or all of, the interaction centers of the interaction center chain to generate a force field comprising short-range interactions, thereby producing a data set representing a three-dimensional model structure of the target protein; and

(b) outputting the three-dimensional reduced protein model to an output device or a storage area.

15. (currently amended) The method of claim 14, wherein producing the data set representing a three-dimensional model structure of the target protein comprises determining side chain center of mass positions of amino acid residues of the target protein by generating a force field comprising short-range interactions that reflect secondary structure propensities and short-range packing biases ~~at least one interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds~~.

16. (currently amended) A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

(a) generating input data for the computer comprising:

(i) inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence; and

(ii) by way of executable code, directing the processor to produce from the alignment a three dimensional reduced protein model comprising representations of side chains of amino acid residues comprising a target protein wherein said representations of side chains of amino acid residues are converted to interaction centers and each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and each interaction center is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain, which is projected onto an underlying cubic lattice to produce a projected chain of interaction centers, and then secondary constraints and/or tertiary constraints are applied to a subset of, or all of, the interaction centers of the interaction center chain to generate a force field comprising short-range interactions, thereby producing a data set representing a three-dimensional model structure of the target protein; and

(b) outputting the three-dimensional reduced protein model to an output device or a storage area.

17. (previously added) The method of claim 14 or claim 16, wherein the executable code comprises instructions for:

connecting said interaction centers by virtual covalent bonds, wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain.

18. (previously added) The method of claim 17 wherein the executable code further comprises projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain on interaction centers.

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19. (previously added) The method of claim 18 wherein the executable code further comprises applying secondary constraints and/or tertiary constraints to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

20. (previously added) The method of claim 14 or claim 16, wherein the executable code comprises instructions for:

(a) connecting said interaction centers by virtual covalent bonds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain; and

(b) projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain on interaction centers;

(c) applying secondary constraints or tertiary constraints, or, secondary constraints and tertiary constraints, to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

21. (previously added) The method of claim 14 or claim 16, wherein the target amino acid sequence comprises a sequence of less than all of the amino acid residues of a protein.

22. (previously added) The method of claim 14 or claim 16, wherein the target amino acid sequence comprises a sequence of all of the amino acid residues of a protein.

23. (previously added) The method of claim 14 or claim 16, wherein the interaction center comprises a pseudoatom representing a center of mass of a side chain.

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Please add the following new claims:

24. (NEW) The method of claim 15, further comprising combining the force field with a small number of long-range harmonic constraints to generate a three-dimensional model structure of the target protein.

25. (NEW) The method of claim 14 or claim 16, wherein the method is iteratively repeated to generate a three-dimensional model structure of the target protein.